Modeling of Complex Material Systems in Extreme Environments for Space Technology

Completed Technology Project (2012 - 2016)

Project Introduction

Among the many enabling technologies of space research is the design of materials which are stable in the environments of interest for a given application. At the cutting edge of material design are complex materials: hybrids, composites, and alloys whose constituents and processing details can lead to a wide range of properties. The design of a complex material can be focused towards specific or multiple applications, and tailored to meet the requirements of a given mission. Hybrid materials are defined by two distinct constituents mixed at the molecular level, usually an inorganic phase intermixed with large organic molecules. The field of nanocomposites intersects somewhat with the field of hybrid materials, though composite materials are typically distinguished by larger spatial separation between constituents. Complex materials may offer the properties of two different materials in parallel, with additional effects due to chemical interactions. Furthermore, alloys and hybrids can form the constituents of advanced composites. The possibilities are extremely numerous in designing complex materials, to the extent that experimental trial and error becomes impractical and costly. We propose that material simulation techniques may have much to offer in the design of complex materials, from high-throughput material selection to detailed observation of chemical processes in a given environment. Here, we focus on the development of atomistic (atom-by-atom) models for complex materials in extreme environments. Empirical models, in which atoms are assumed to exhibit parameterized interatomic potentials, often lack the transferability necessary to explore extreme environments. This is because they are typically fit to a set of properties which may or may not be reliable outside of the range of fitting. For this reason, it is important to employ quantum mechanical methods as closely as possible. However, complex material systems naturally require a large number of atoms to construct a representative unit, presenting a problem for quantum methods in which computation time scales at best quadratically with system size. Density functional theory (DFT) calculations have become widely utilized in material simulations because of their remarkable ability to reproduce measured quantities. DFT calculations are limited to a few hundred atoms on a high-performance system. This may be enough to study the ground state properties of complex material systems, but DFT is known to misrepresent certain interactions that are likely relevant to the problem of complex materials design, such as van der Waals (vdW) bonding. Empirical extensions to DFT are commonly employed to achieve resolution of such misrepresented effects. Examples include empirical corrections to quantum models and/or application of known macroscopic properties to shrink the representative unit for atomistic calculations. Such approximations will certainly be necessary to approach the problem of modeling complex materials, especially in consideration of time-dependent processes in extreme environments. We consider one important application in space technology: design of hybrid materials for thermally protective ablators during atmospheric entry. Engineered hybrid materials are attractive for this application, as there will be a very specific set of

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Organizational Responsibility

Responsible Mission Directorate:

Space Technology Mission Directorate (STMD)

Responsible Program:

Space Technology Research Grants

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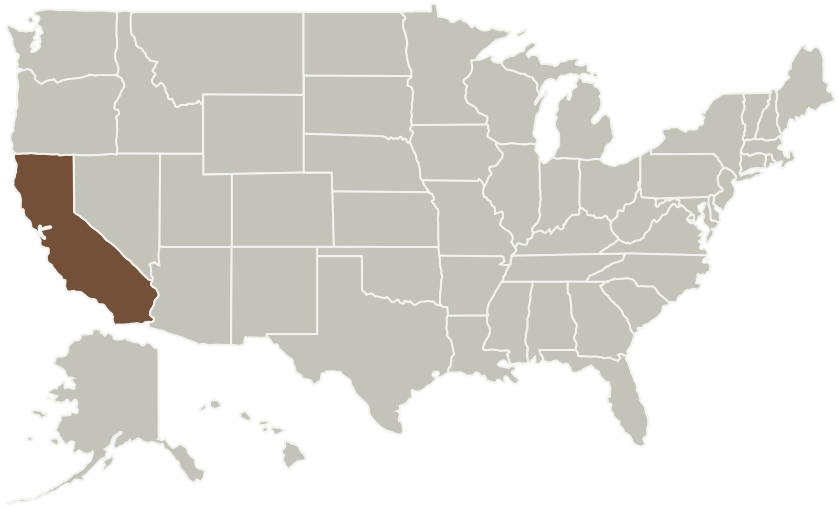
requirements for a given ascent. Mechanical stability and precisely tuned ablation characteristics are desirable, and there is potential to engineer enhanced optical properties (at atomic as well as photonic scales) to reduce radiative heating. The actual thermal, mechanical, and optical design goals will vary depending on the atmosphere and vehicle of interest. A computational model could be used first to select candidate materials for a given application, then to isolate and tune the relevant degrees of freedom for the intended purpose, and finally to expand the scale to an actual device and inexpensively test the design.

Anticipated Benefits

We consider one important application in space technology: design of hybrid materials for thermally protective ablators during atmospheric entry. Engineered hybrid materials are attractive for this application, as there will be a very specific set of requirements for a given ascent. Mechanical stability and precisely tuned ablation characteristics are desirable, and there is potential to engineer enhanced optical properties (at atomic as well as photonic scales) to reduce radiative heating. The actual thermal, mechanical, and optical design goals will vary depending on the atmosphere and vehicle of interest. A computational model could be used first to select candidate materials for a given application, then to isolate and tune the relevant degrees of freedom for the intended purpose, and finally to expand the scale to an actual device and inexpensively test the design.

Primary U.S. Work Locations and Key Partners



Project Management

Program Director:
Claudia M Meyer

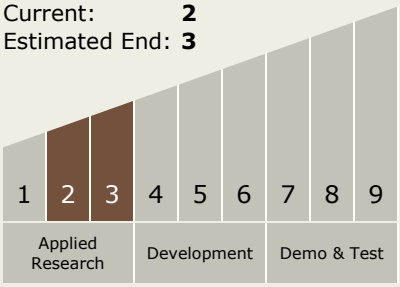
Program Manager:
Hung D Nguyen

Principal Investigator:
Evan Reed

Co-Investigator:
Lenson Pellouchoud

Technology Maturity (TRL)

Start: **2**
Current: **2**
Estimated End: **3**



Technology Areas

Primary:

- TX12 Materials, Structures, Mechanical Systems, and Manufacturing
  - TX12.1 Materials
    - TX12.1.1 Lightweight Structural Materials

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Primary U.S. Work Locations
California

Project Website:

https://www.nasa.gov/directorates/spacetech/home/index.html